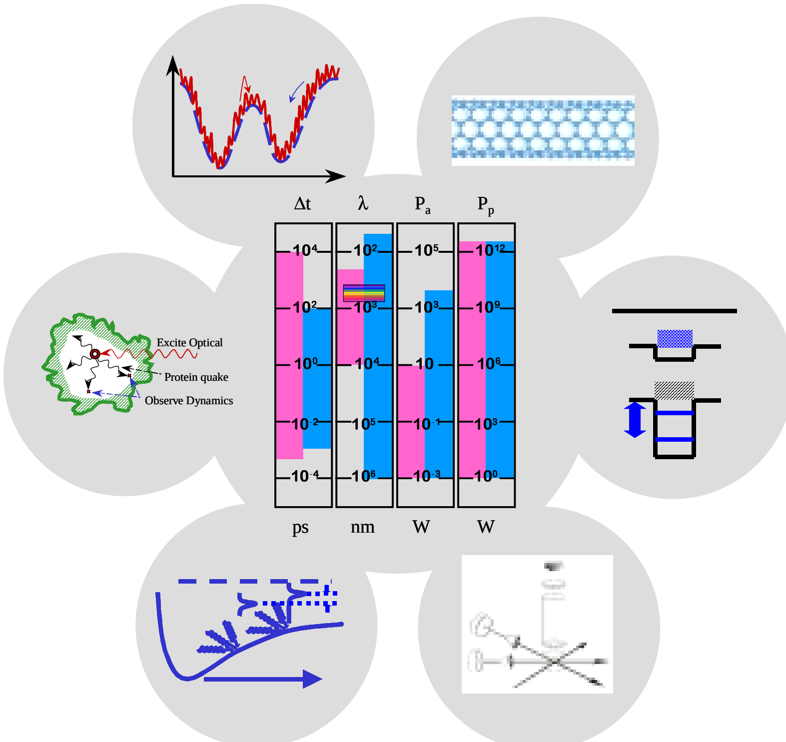
Scientific Frontiers with Accelerator-Based Lasers

May 1, 2001



The report of a meeting held October 12–13, 2000, at the Wyndham Hotel and the American Association for the Advancement of Science, Washington, D.C.

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Contents

Executive Summary

Recent years have brought dramatic advances in laser technology. However, there are critical scientific opportunities at the research frontiers of biology, medicine, chemistry, and materials science that are exploitable only by going beyond the present performance limits in wavelength range, mode quality, tunability, peak power, and average power. Many of these opportunities are ripe for development using the new generation of Free-Electron Lasers (FELs) and upgrades of these FELs based on new advances in technology.

At the forefront of many disciplines are:

1. Dynamical studies that span the time-frame from initial photo-excitation to the time-evolving roles of the electronic quantum and vibrational structure of matter. These studies at the interface of photonics and electronics span:

    - Atomic, molecular, and chemical science using quantum control.
    - Condensed matter science involving fundamental studies of conductivity and magnetism, including synthetic materials and devices.
    - Biology and medicine, including the energy landscape for complex systems of proteins.

2. Studies of nonlinear phenomena that drive new materials and devices such as synthetic quantum structures, novel magnetic materials, superconductors, and new forms of matter such as novel nitrides and carbon nanotubes.

An opportunity exists for the USA to move into a world-leading position by developing FEL facilities to address unique new areas which are currently inaccessible using existing lasers. To accomplish this will require a commitment to the development of user facilities, and an aggressive campaign to nurture users similar to that practiced for synchrotron radiation. Particular areas of focus are the far-IR, the UV-VUV, and rapidly tunable, high-mode-quality, high-power, tunable mid-IR.

Introduction

This broad-based report resulted from a meeting held in Washington October 12–13, 2000, which was charged with identifying the science drivers for light sources below 100 eV. It was a timely meeting for two reasons. First, there have been significant scientific developments since these areas were addressed in the National Research Council's 1994 report "Free Electron Lasers and other Advanced Sources of Light: Scientific Research Opportunities". Second, the 1999 "Leone" report on "Novel, Coherent Light Sources" from the Department of Energy's Office of Science, Basic Energy Sciences Advisory Committee, emphasized x-ray applications. We attempt here to update the situation in the IR-VUV spectral region.

Fifty-two people attended the workshop. (See appendices.) Six specialized groups discussed the scientific frontiers in:

Biological Physics

Medical Physics

Atomic and molecular science

Condensed Phase Dynamics

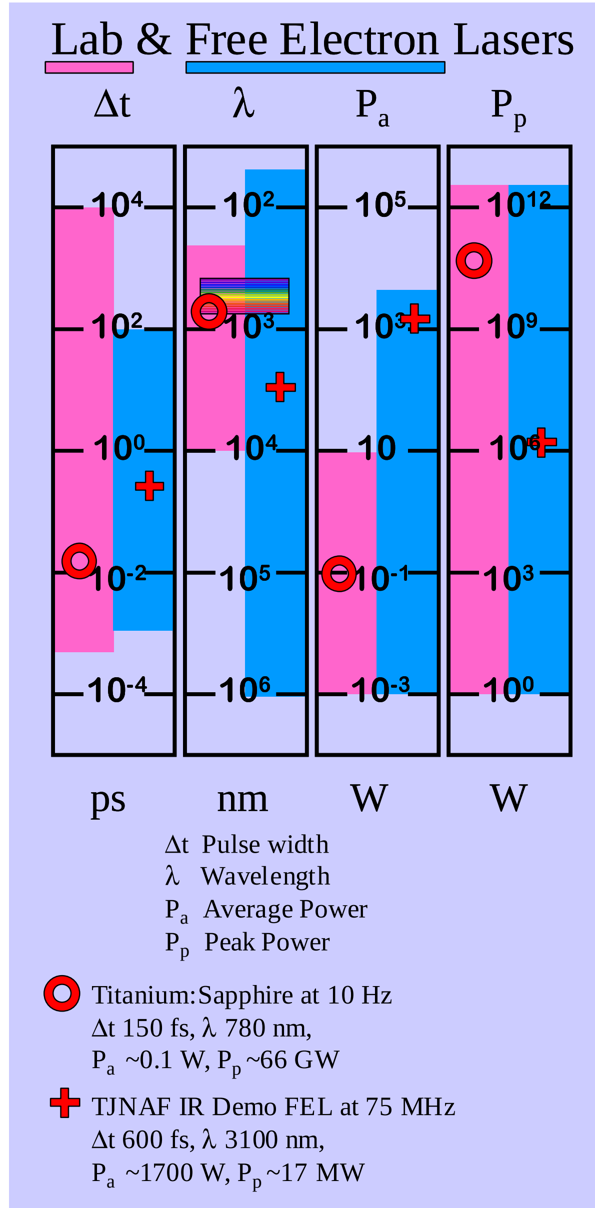
Nanofabrication and Growth Characterization

Gas-Phase Chemical Physics

In the report that follows we present the findings of each group in a format that first defines the scientific drivers, then reports the impact on technology and society, and ends with the source requirements.

Roles of Free-Electron Lasers

This report attempts to define the critical scientific roles that Free Electron Lasers could fulfill. Generally these machines are complex facilities that may be located some distance from a researchers home laboratory, hence they will be most useful only in cases where alternative sources do not exist, and the scientific need is compelling. We graphically compare the approximate parameters from routinely available laboratory laser systems with FEL's in the figure to highlight the differences in a way that suggests possible opportunities to be explored. One should not form the impression that any arbitrary set of parameters can be demanded from either type of source. For example the parameters from a rather modest lab based Titanium Sapphire system (circles) are compared with one set of running conditions for the TJNAF IR-Demo FEL (crosses). The range of visible light is also included on the wavelength scale for reference. In each of the sections of the report we have included similar figures. An extra band has been added to each to illustrate the range of requirements for the science they describe. While these figures provide a useful touchstone, they fall far short of capturing the entire range of the parameter space that may enable an entirely new scientific endeavor. They do however, like this report, represent a place to start.

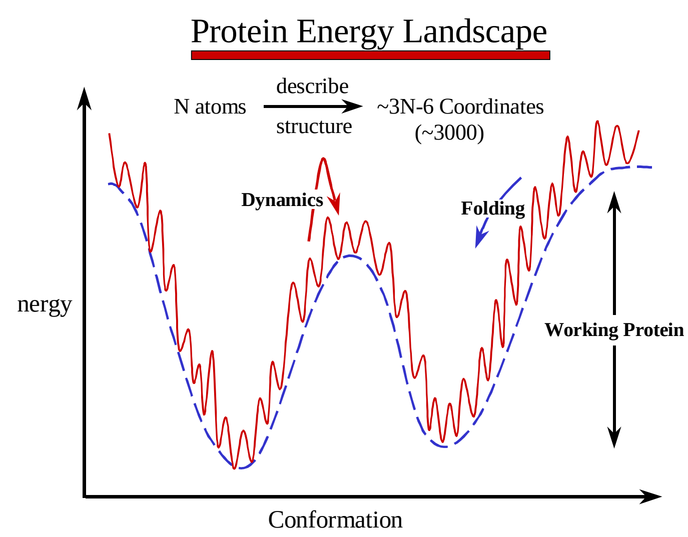


1.1 Biological Physics

Frontiers of biological physics

We identified two main areas where high-brightness accelerator-based lasers can make major contributions to biological physics: protein structure/function studies and molecular cell physiology. We first discuss protein structure/function studies.

At present, no protein is fully understood in a dynamic way. A major forefront in biological physics is establishing a quantitative connection among the structure, energy landscape, dynamics, and function of a few selected proteins and discovering the general concepts and laws that govern protein function. Protein structures are currently determined at a surprising rate. However, these structures show the proteins in a stationary state. In contrast, the working proteins assume structures that can be very different from their "textbook" pictures. Determining structures of proteins at work is a major challenge that will remain a forefront for many years.



Major progress in essentially all subfields of physics was made through the determination of the energy levels. In biomolecules, the energy levels are generalized to an "energy landscape": a given primary sequence does not fold into a unique tertiary structure, but can assume a very large number of related, but in detail different, structures. The ensemble of these structures is described by the energy (or conformation) landscape. While some features of the energy landscape are known for a few proteins, a detailed description is lacking.

Proteins are dynamic, functional molecules. The dynamics are transitions in the energy landscape and are crucial for protein function. Protein folding is one specific aspect of the dynamics, but understanding dynamical processes is also critical for elucidation of the function of folded proteins. The ultimate goal is the quantitative description of the function of a protein. This goal, a major forefront, will require close collaboration among biologists, chemists, and physicists and involve experiment, theory, and computation. Powerful photon sources that are broadly tunable throughout the x-ray, UV, visible, and IR regions will be essential to this work, because of the huge range of the energy levels of conformational states that play a role in protein dynamics. All the energy levels, whether it be the large-scale collective modes in the far IR or the electronic levels in the UV range, are coupled together in a complex manner, and it is this coupling that is critical to protein action. The parameters needed to do multiwavelength pump/probe experiments are challenging but achievable: we need on the order of 100 microjoules in a picosecond micropulse to achieve substantial level pumping, and because the signals in protein dynamics are typically small we need at least a 1 kHz repetition rate of low-amplitude-variance (less than 1% pulse-to-pulse) micropulses. Single micropulses are critical to avoid sample heating, so although the average power needed per experimental line is low (0.1 W) these micropulses must be selected out of a (typical) 20 MHz train of micropulses, so the input beam energy is quite high, 2 kW.

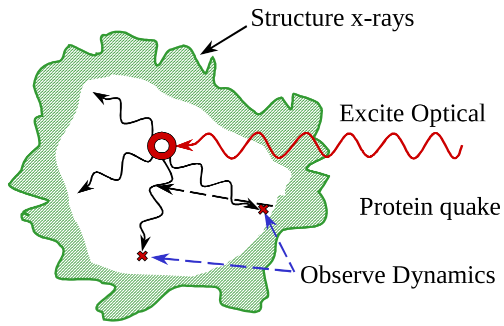
Most protein research so far has been performed on purified samples in vitro. However, experiments on proteins in a single cell and measurement of the effect of protein-protein interactions will extend the forefront even further. The emerging field of proteomics, in part, addresses these issues. New techniques—such as InfraRed Matrix-Assisted Laser

Desorption Ionization (IR-MALDI) mass spectrometry, and far-UV time-resolved circular dichroism and Raman scattering—offer means to examine such interactions and require powerful, pulsed light sources that can be tuned to any wavelength across a broad spectrum. One forefront of this research is understanding molecular mechanisms of MALDI in order to capture the richness of absorptions in the mid-IR. These experiments again are energy- and power-intensive since they ablate samples from surfaces, so we need again 100 microjoules/micropulse and a high repetition rate of single micropulses to achieve high sample throughput over an array of spots. Circular dichroism and Raman measurements have already been extended to the nanosecond time range using conventional lasers for wavelengths > 300 nm, but the maximum impact for dynamic structural biology depends on moving to the far UV where the amide groups of proteins absorb. In these examples, additional information may be acquired using the nonlinear absorption effects that come from high-power lasers. Once again, the power requirements are substantial due to the necessity of high-energy single micropulses at a high repetition rate.

IR-MALDI:
InfraRedMatrix-Assisted Laser Desorption Ionization mass spectrometry

Molecular cell physiology is another forefront. Examples include the production of DNA and protein photoproducts and resultant effects on cells, tissues, and organisms. The high intensity and wide spectral range of FELs will permit measurements of such effects in regions such as the near UV (320–400 nm), where the cross sections for damage are low, and the far UV (< 240 nm), where existing continuously tunable sources have inadequate intensity. The necessity in biology of exciting many samples at once to obtain good statistics in an inherently noisy sample means at least 100 W/m^2 over square-meter areas will be necessary. The quantitative relationship among structure, dynamics, motility, and

Proteins and Photons



cellular function is poorly understood. Advances in genetics, optics, and laser-tissue interactions present opportunities for real-time, in vivo imaging of transgenic cells and tissues. Molecular dynamics and cell motility play essential roles in cell physiology. The programmed movement of nuclei and then cells in developmental biology is highly reproducible and symmetric. Whole-volume, time-resolved in vivo imaging would bring great benefit. Better understanding of the mechanisms underlying patterned motion as well as laser microsurgery and laser perturbation of cell physiology hold promise for medical sciences and biotechnology. These again are high-average-power/high-brightness applications because single micropulses that do not excite the vapor plume are critical.

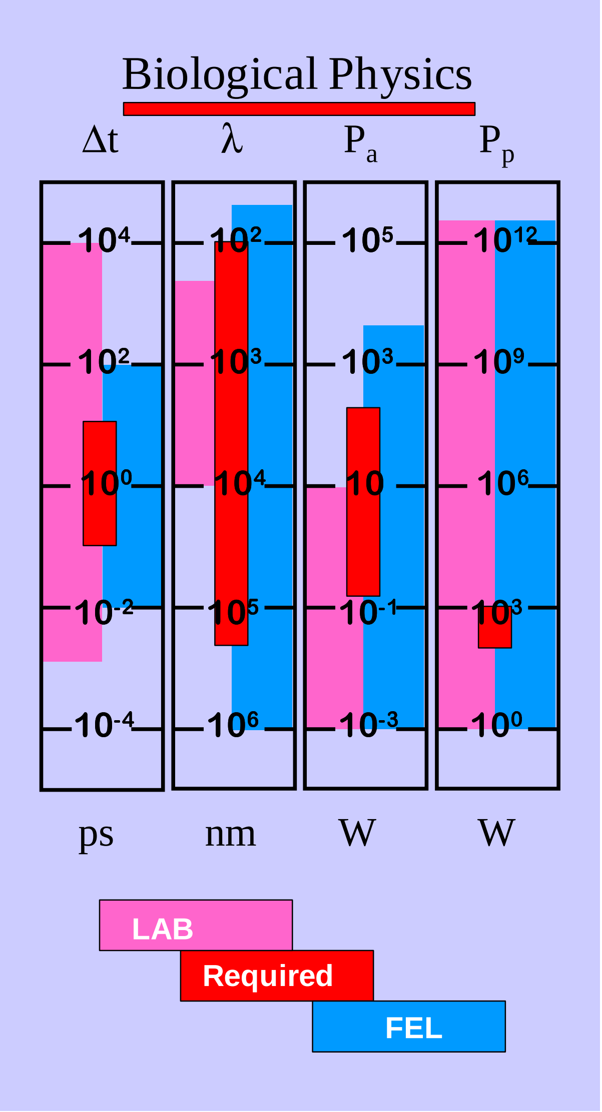
Impact of new biological physics research on science, technology, and society

The impact of new insights and solutions to fundamental problems on science, technology and society is unpredictable. In the case of biological physics, however, a few predictions can be made with some confidence. A quantitative understanding of the function of proteins and cells will advance biotechnology, and permit the creation of better drugs, leading to better quality of life. Use of new light sources for the experimental work will improve capabilities to diagnose and treat diseases with light. The understanding may also lead to more general insights into the workings of complex systems, and to the construction of biological computers.

Source requirements for biomedical research

The development of new capabilities from accelerator-based lasers depends crucially on the electron beam quality. The potential exists for wavelengths shorter than 1 Å, as well as gamma rays via Compton backscattering. The potential also exists for sub-100-fs pulses, variable macrpo-pulse structures, variable polarization, and average powers exceeding 10 kW, both in order to enable 1 kHz single high-power micro-pulses as we have discussed and later to provide the promise of serving multiple users with multiple colors, essentially jitter-free. We stress that a multiple-user facility is critical because of the wide range of experiments that must be done and the different optical configurations necessary. For example, measurement of protein energy landscapes calls for continuous wavelength tunability on the minute time scale, variable pulse widths from 10 fs to 100 ps, variable pulse repetition rate from single pulses to 3 GHz, and synchronization of multiple colors through the UV/visible-IR/far-IR range. It should be recognized that the optical quality of the light will constrain the applications research. While many experiments do not require the highest optical quality, other classes of experiments, such as optical holography or coherent control, are more demanding.

Brightness is the photon intensity per unit source size, divergence, and spectral bandwidth. The high photon flux that some FELs can produce, i.e., the numerator of the brightness formula, is critical for some of the unique experiments that are made possible by FELs. Other experiments depend critically on the small values achievable in the denominator of the brightness formula. Small source size and small divergence are



critical for biological and medical imaging, which can be extended into new spectral regions by FELs.

Short pulses are critical for many of the important biological applications, including multiphoton-induced photochemical and radiological reactions, pump-probe studies of excited states and reaction intermediates, time-resolved circular dichroism and Raman spectroscopy, and other experiments in dynamic structural biology.

Spectral resolution (small spectral bandwidth) is also critical in experiments to determine the energy landscape of proteins, nucleic acids, and their complexes. It is typical in biology for the spectral transitions to be inhomogenously broadened, so elucidation of the underlying energy states requires hole-burning experiments. Specific experiments requiring high spectral resolution include studies of energy transfer in proteins probed by IR radiation and far-UV, time-resolved Raman scattering. In the case of the mid-IR experiments as an example, although the amide I band is about 40 cm^{-1} wide, the relaxation times measured indicate that the transform-limited widths are about 10 cm^{-1}, pointing out the need to have narrow linewidth excitation.

1.2 Medical Physics

Frontiers of medicine using lasers

Medicine has moved and will continue to move toward minimally invasive procedures for both diagnosis and treatment. Pharmacological surgery (e.g., where activation of a chemotherapeutic agent could kill only malignant cells, superior to a surgeon's scalpel excising a tumor) and the stimulation of other targeted effects at any depth within the body will become essential technology for the advancement of medical practice.

The information we desire must be acquired on an anatomical, functional, and molecular level by fusion and correlation of imaging data, using light, x-rays, fMRI, MRS, PET, and SPECT, down to the microscopic/cellular level.

fMRI: functional Magnetic Resonance Imaging
MRS: Magnetic Resonance Spectroscopy
PET: Positron Emission Tomography
SPECT: Single Photon Emission Tomography

We propose changing the paradigm in medicine to allow for unique site- and time-specific ways of triggering chemistry in the body when and where one needs it.

- Photobiology will allow us to track information from the gene to the message to the protein in order to demonstrate that drugs reach the tissues of interest and have the desired effects in those tissues. We need to be able to monitor movement of intracellular and intercellular molecules to a specific site and to follow the downstream response in the tissues.

- We must be able to detect site-specific binding and pharmacological actions of drugs.

Impact of new medical research on science, technology, and society

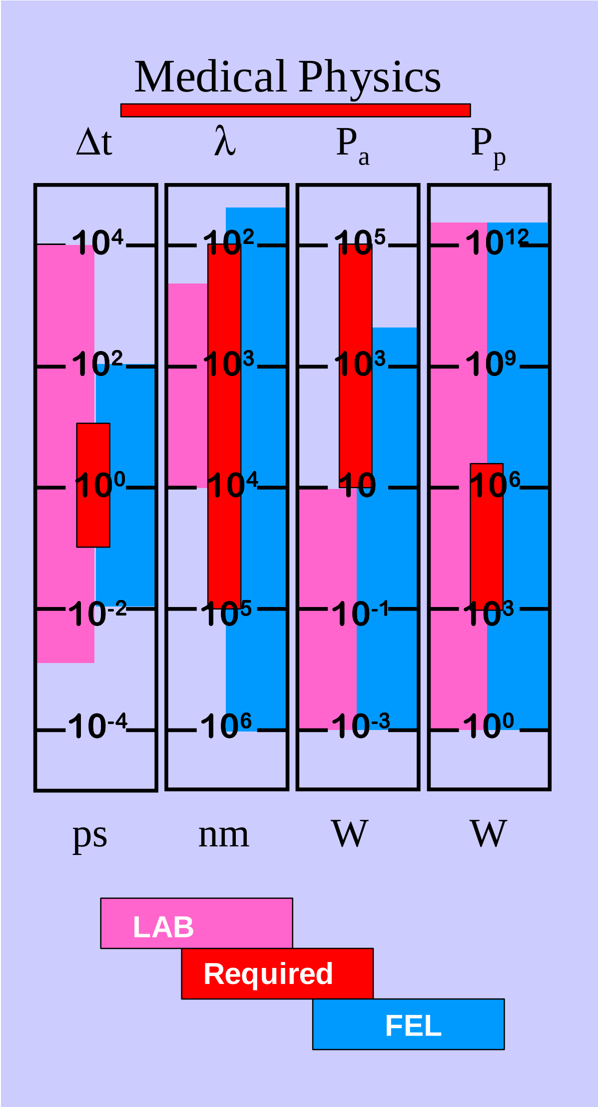
Many novel approaches to medical treatment are enabled by tunable, very high brightness light sources. These include more rapid drug development, photo-activation of new drugs, precision and targeted surgical procedures, new skin treatments, better treatment of cancer, autoimmune, and cardiovascular diseases, and better tools for biomedical research in general. However, new techniques in medical science impact not just quality of life. There has been a progression toward complexity in medicine which has also inflated costs. There is a strong desire to develop new techniques which simplify processes using novel approaches while making treatments more palatable for patients.

The potential impact on society also includes the potential spin-off of smaller photon sources for specific diagnostic and treatment applications.

Source requirements for medical research

To understand these processes, we need high-power, narrow-bandwidth (1–5 nm), variable-pulse-width light sources that are tunable to interesting but not-yet-available wavelengths (e.g., near IR to 400 nm, and 15–50 keV x-rays) and capable of femtosecond operation (10–1000 fs).

These sources would allow stimulation of multiphoton processes within cells at depth. The multiphoton/multifrequency capability would assist us in our understanding of photobiology in the intact organism.



With new sources come other needs, which include:

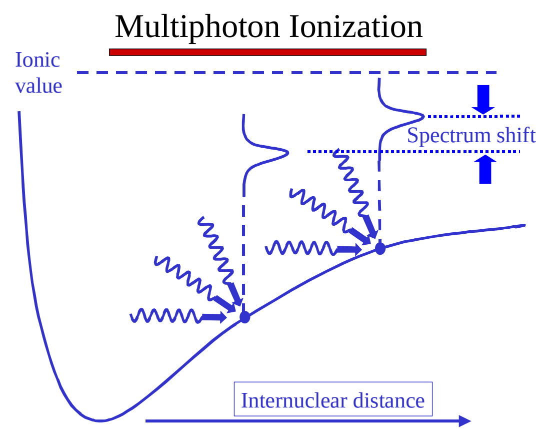
- We must improve delivery systems to bring both currently available techniques (like photodynamic therapy) and next-generation multiphoton/UV techniques to the tissues with minimally invasive technologies to better service treatment and diagnosis of epithelial tumors (skin, gut, airway, and ovarian tumors) that are now accessible to light, but also to extend the benefits of lasers to those solid organs now considered relatively inaccessible.
- We need to extend our capabilities in high-resolution, functional noninvasive imaging through endoscopically delivered multiphoton UV or externally delivered monochromatic x-rays with, for example, heavy metal tagged site-specific agents.
- We need significant improvements in sensitivity and resolution of x-ray and optoacoustic detectors.
- We need to understand the nature of molecular and cellular damage generated by such sources in different spectral regions, particularly the near UV (400 to 320 nm) and far UV (<240 nm), where, respectively, conventional sources are inadequate due to low absorption cross sections and insufficient source intensities.
- We need to determine if delivering UV and ionizing radiation in picosecond pulses affects the type, probability inductions, or distribution of the lesions induced in DNA, RNA, and protein compared to conventional "dc" irradiations.
- These new photon sources must reside at multidisciplinary facilities (not necessarily large plants, but unique in what they offer).
- The facilities need to be integrated with mainstream biomedical research with classical dedicated biomedical research support facilities.

2. Atomic and Molecular Science

Frontiers in atomic and molecular science

Atomic and molecular science has already made major advances in studies of dynamical processes and high-intensity processes. Subpicosecond sources can view atomic motion during a molecular vibration. Intensities above 10^{20} W/cm^{2} are approaching the magic intensity that would spark the vacuum. But the ultimate advances—the ideal fast atomic probe, and a laboratory study of general relativity (which might include a look into the higher dimensions envisioned by string theories)—still require a quantum leap in our technology.

The ultimate dynamic atomic probe would excite inner-shell electrons, rather than valence electrons. Then one might expect small spectroscopic shifts that could be easily interpreted, just as near-edge x-ray absorption fine structure (NEXAFS) is now routinely used to characterize materials on a much slower time scale. As an example consider the dynamics of molecular iodine studied via multiphoton, core electron excitation. Iodine is one of the standard prototypes for pulse/probe studies because it has a strong visible "pump" excitation. In this example a 4d electron would be photo-ionized by five-photon absorption from a 10 eV source to probe one of the iodine atoms as it vibrated after an initial visible pump. VUV multiphoton absorption has seldom been done, because of the immense effort required to produce even a single (mostly untunable) source. But an easily tunable, multiphoton VUV probe would have considerable benefits over more traditional techniques. Visible probes can only see the valence electrons, and they suffer shifts far in excess of the splitting between levels as the molecule vibrates. Inner-shell



electrons have smaller, chemical shifts that are perfect for identifying atomic structure. If they also show a time-dependent chemical shift as the molecule dissociates, they will provide a perfect picture of the dynamics. One might try to use high-order multiphoton excitation to reach these inner shells, but intense visible lasers produce complicated "dressed atom" shifts that have made them useless for inner-electron spectroscopy to date. The fundamental questions are, how deep must one probe into the inner shells, and how few photons can one use to attain the ideal combination of small, identifiable chemical shifts? Current third-generation x-ray sources cannot reach the subpicosecond timing requirements necessary to probe intermolecular vibrations, nor are they a good match to the repetition rate of ultrafast "pump" sources. An intense 10 eV source would simultaneously generate the subharmonic to make a perfectly timed pump source.

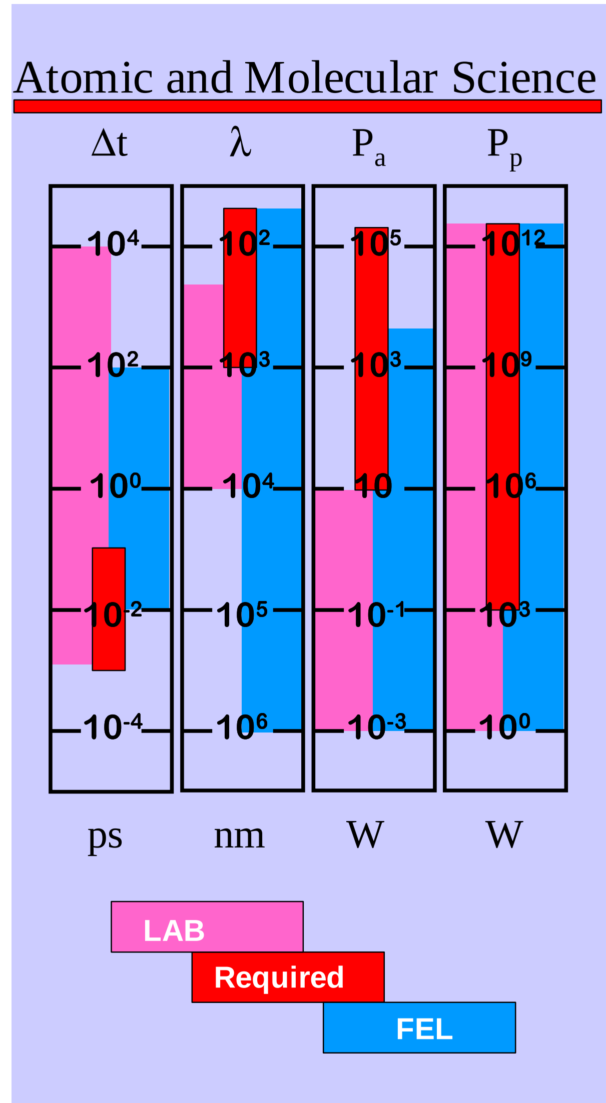
On the high-intensity frontier, the most important class of experiments may be to measure the Hawking/Unruh radiation from a free electron accelerated by a laser field. Hawking first theorized that the region near a black hole radiates as a blackbody with a temperature proportional to the local acceleration. Unruh extended this idea to show that an accelerated charged particle will also emit this radiation. Since this is a general relativistic effect, it could probe some of the dimensions of space-time—even those which we may not normally see. The spectrum of this radiation might allow us to see outside the normal electromagnetic spectrum. An electron will be (periodically) accelerated to a relativistic speed by a laser focused to a tight spot size far exceeding any other laboratory electric fields. When accelerated by these fields, the electron will generate Unruh radiation.

Impact of atomic and molecular science on science, technology, and society

Fundamental studies of atomic and molecular species underpin much of the work on condensed phase systems and in chemical dynamics, and hence impact our technology. The development of an intense VUV source and the associated optics required for it could form the basis technology for the next generation of shorter-wavelength photolithography. The revolution in microscopy, due to ultrafast sources enabling two-photon microscopy, will be significantly advanced by extension into the UV (particularly if the multiphoton core probe is successful). Advances in our understanding of the influence of intense fields will likely lead to new discoveries and new technologies. If intense lasers can create a laboratory for general relativity studies, then the impact on science would be immense. This would truly cause a paradigm shift, as it would be a way to study quantum gravity or the possibility of compacted dimensions.

Source requirements for atomic and molecular science

Current bench-top sources give millijoules in 100 fs at 800 nm. Some power exists in harmonics, but UV output is low due to the materials that are typically used. Needed are millijoule pulses at 5–10 eV in 100 fs, shaped pulses, at high repetition rates. For the experiments described above, the high energies can be produced in a high-Q external cavity, since the experiments themselves are nondissipative.

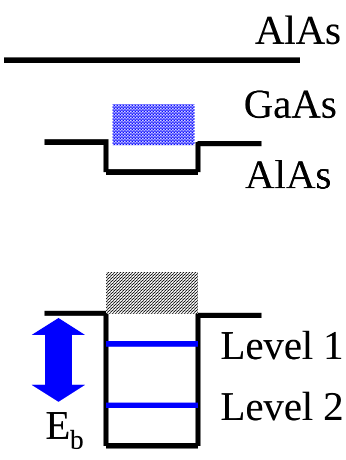


3. Condensed Phase Dynamics

Frontiers in condensed phase dynamics

At the forefront of condensed phase studies are fast time-resolved dynamical studies of the evolution of the behavior of electrons and phonons, and studies of the nonlinear response of systems that drive novel phenomena. In particular, studies of the evolution of the frequency-dependent conductivity and phonon dynamics in perturbed systems and the interplay between the two are critical to a fundamental understanding of the macroscopic behavior of materials.

Regarding specific systems, the dynamics of nanoparticles are different from those of the bulk, and the scaling leads to quantum effects, which are accessible to study given improved source characteristics. Examples are small samples of novel materials, including exotic structures with engineered properties that take advantage of quantum behavior, and small perturbations induced in time-resolved studies. The aim is to be able to use coherent control to drive selected quantum excitations. More specifically, there is a desire to probe the behavior of a single quantum structure, to probe intraband dynamics, to study coherent coupling of quantum dots, and to characterize energy levels at interfaces. With an appropriate light source, one can also study photon-assisted tunneling through barriers of both electrons and ions.



Schematic of a quantum dot.
Top: Physical structure
Bottom: Energy Levels

Defects often dominate in material properties, and theoretical understanding and modeling are not well refined particularly for anharmonic potentials, an example being hydrogen defects in Si. IR relaxation and dephasing lifetimes in the bulk, at interfaces, and on surfaces of hard, soft, and biological material are therefore critical to the development of models and fundamental understanding.

Surfaces and interfaces, including adsorbate bonding and dynamics, play a key role in material interactions. The systems are difficult to study because of the dilution problem; however, bond-breaking and desorption experiments—vibrationally induced, two-color (UV/IR) characterization of energy surfaces during desorption—could play key roles in revealing the underlying physical mechanisms and processes. Surfaces can be further studied via nonlinear sum/difference frequency-mixing and harmonic-generation processes that occur because of the symmetry breaking, and that can allow the study of biological lipid bi-layers, polar molecules, oxide growth on semiconductors, and carrier injection and transport at surfaces. Finally, electronic quantum structure can be explored in a novel way, using two-photon photoemission—particularly if both photons are tunable so that intermediate states can be revealed.

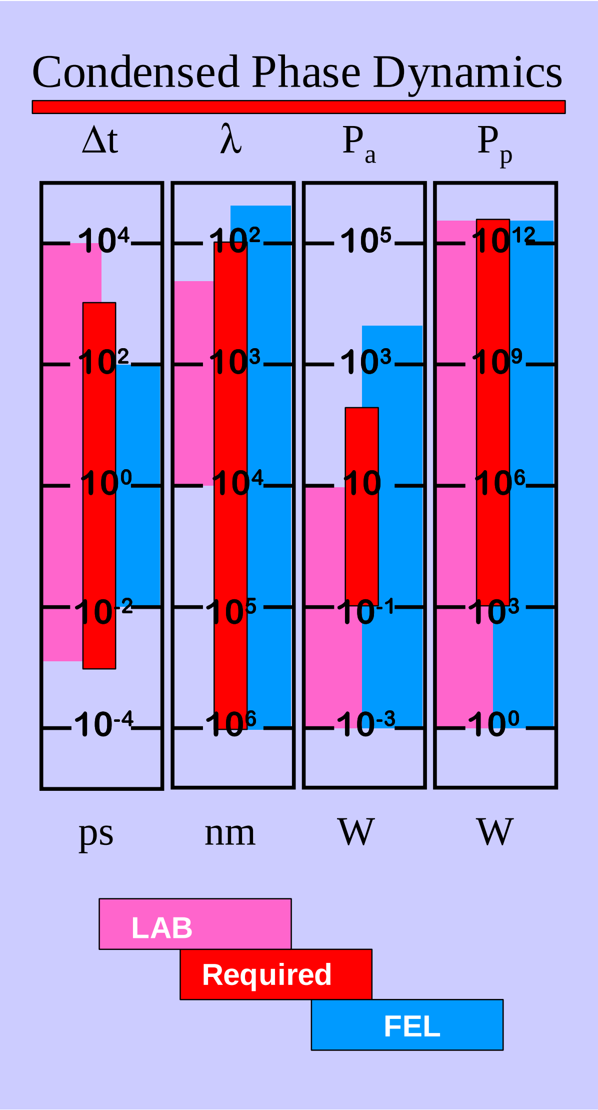
Finally we note that novel imaging of biological and semiconductor microstructures can be performed using photon-echo techniques which themselves involve nonlinear THz interactions and in which FELs are expected to play a major role.

Impact of condensed phase dynamics on science, technology, and society

The primary impact of this field on technology is contributions to devices involved with information technology, including optical switching, THz technology using coherent control of electronics, and the electronic-to-photonic transition. Additional applications will be in analytical techniques, including dynamical spectral microscopy, single-quantum structure analysis, and subcellular biology.

Source requirements for condensed phase dynamics

Broad tunability with coverage from the far IR through the UV region of the spectrum is most important. Sources must be intense, with excellent pulse-to-pulse stability. Pulse amplitude, phase, frequency, length, and chirp control will become increasingly important. Sources must be coupled to other laser or white-light sources for two- or more-color experiments. In addition to the source characteristics, additional on-site infrastructure is needed, including conventional spectroscopic and characterization tools as well as materials growth and fabrication facilities.



4. Nanofabrication & Growth Characterization

Frontiers of nanostructure fabrication

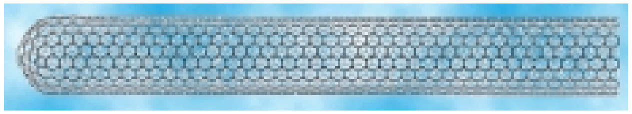
Efforts at the frontiers of nanofabrication and growth characterization are aimed at understanding the underlying physics and chemistry in directed assembly of nanometer-scale structures with novel properties. Current challenges in nanotechnology include achieving high sample uniformity in size and space, especially for asymmetric material structures, adding metals and insulators to the mix of materials, adding functionality with nanometer-scale spatial resolution, assembling nanocrystals into nanostructures and nanodevices, and understanding growth processes on the nanometer scale in real time.

Laser processing with conventional Nd:YAG and excimer sources begins with electronic excitations which then transfer their energy via electron-phonon coupling to the lattice. The long pulse duration of conventional lasers implies that all processing is occurring at thermal equilibrium. The low average power of conventional lasers gives inadequate throughput for rare processes. Nanofabrication and growth characterization can benefit enormously from the use of FELs because materials can be processed in non-equilibrium regimes with high throughput.

FELs are uniquely suited to many aspects of nanofabrication and nanocharacterization because their tunability implies specificity. They allow target-specific, localized growth modes while the ultrashort micropulse duration optimizes laser-materials interaction. Further, the high average power gives access to rare processes, and allows size scaling (e.g., nanostructure arrays), maximizing throughput. The high peak power can itself be used for nonlinear optical diagnostics that have the same kind of enhanced utility in nanofabrication that they have in photobiology (i.e., low linear absorption and thermal collateral damage, and high specificity). The following paragraphs illustrate how the FEL can benefit this process in several ways.

A critical problem is the area of one-dimensional nanomaterials. The electronic properties of nanotubes, nanorods, and nanowires are crucially dependent on structure and growth mode. They are recognized as a major problem needing vastly better growth processes than presently available. Small bundles of Single Wall Carbon Nanotubes (SWNTs) have the highest strength-to-weight ratio of any known material, with an elastic modulus of ~1 Tpa, which makes them 100 times stronger than steel. According to a U.S. Department of Energy report*, making these materials for practical applications "will require the development of new approaches for high-volume, directed deposition of nanostructured materials. SWNTs, for example, are not useful for structural applications unless they can be grown directly into strong composite structures 1000 times faster than current CVD methods." Theory, computer modeling, and experimental diagnostics of transport and growth phenomena are all needed to fabricate nanostructured building blocks at near-theoretical growth rates.

Single-Wall Carbon Nanotube



*Nanoscale Science, Engineering and Technology Research Directions, U.S. DOE, 1999.

FEL synthesis of one-dimensional nanostructures: Quantum wires and nanotubes are a critical component of nanostructured devices of the future. Laser ablation is the preferred synthesis route to SWCNTs, and FELs could be used to develop the optimal strategy: For example, a high repetition rate permits pumping of the vapor plume, while tunability allows preferred growth modes to be selected by selectively controlling vibrational heating and thus optimizing the laser-materials interaction at the target. In addition, high average power can be used for maximizing overall production rates, while multicolor lasing or multiple lasers (not all ultrafast) can be used to optimize laser ablation as well as for diagnostics. This project could be extended to other one-dimensional structures such as Si, Ge, GaAs, CN, BCN, and WS_2.

Two-dimensional nanostructures: FELs can play a unique role in the synthesis of planar, horizontally structured layers required for complex structures. Pulsed laser deposition with ultrafast energy deposition optimizes laser-materials coupling; tunability permits the most efficient photon energies to be determined and used; a high pulse repetition rate maximizes deposition rates. Additional structuring is possible using laser direct-writing (forward transfer) of nanostructures with the high pulse repetition rate maximizing the raster scanning rate.

In addition, surfaces can be modified or annealed, and the electrical, optical, structural, and mechanical properties of materials such as semiconductors, photovoltaics, and transparent conductors can be tailored. Surfaces can also be prepared for chemical functionality using post-deposition processing.

Cluster-assembled three-dimensional structures: Another possible route to nanocomposite materials and structures is to use vapor-phase nanocrystal formation (already observed) and modification of surface reactivity. Materials of intererest are magnetic nanodots for quantum computing and magnetic memory, encapsulated optically active nanocrystals and nanoclusters, encapsulated nanoclusters for catalytic applications, metal nanocrystals in dielectrics for nonlinear optical elements, and sintered nanocluster-assembled ceramics.

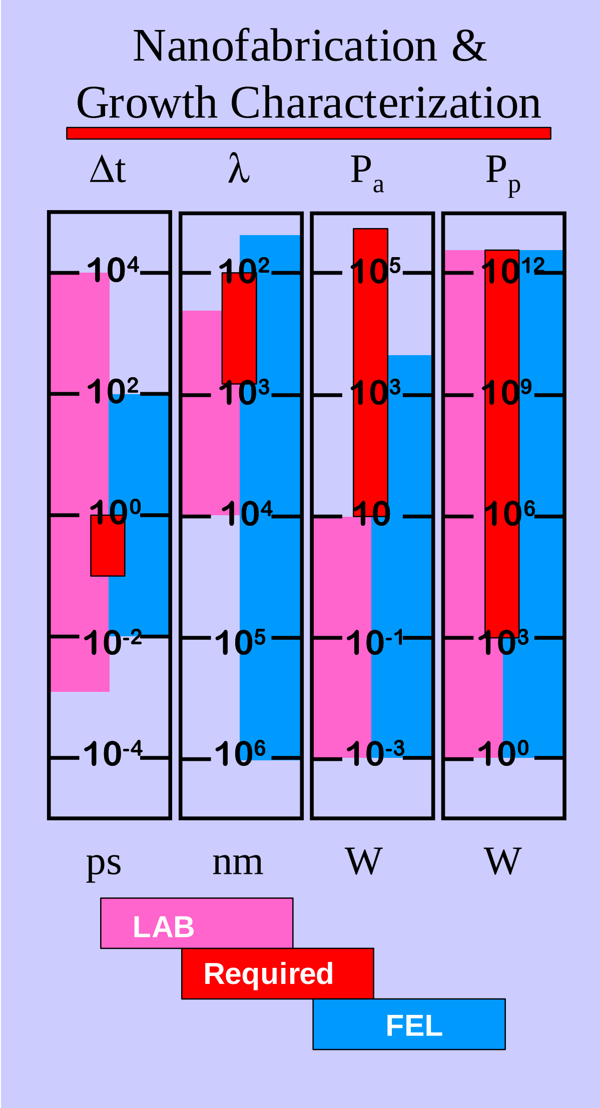
Key points for investigation with FELs are the time scales and mechanisms of enhanced surface reactivity, for example whether it is thermal or activated through a local electronic or vibrational excitation mode. There are key fundamental physics questions involving the evolution of the bulk electronic quantum and phonon structure with size, and the substrate interface dynamics. These relate to the effect of thermalization of nanocluster energy on the growth process.

Impact of nanofabrication on science, technology, and society

Although nanophase materials are already being incorporated into materials processing in a number of different areas, the expectations for a new industrial revolution based on the science of the very small really hinges on the assembly of devices and systems based on nanostructures. The major impacts known so far include medical uses of nanoscale structures (as fluorescent probes), molecular electronics, and optical switching elements in fiber communications.

Source requirements for nanostructure fabrication

- High spectral brightness, coupled with broadband tunability for specific processes and resonances, and the ability to rapidly scan the wavelength.
- High intensity and pulse-repetition frequencies are required for low surface coverages, and for systems with low interaction cross sections.
- Two colors are required for some pump-probe experiments.
- There is a requirement for a user facility with additional conventional light sources, standard and custom-made materials synthesis tools and real-time, spectrally and spatially resolved microscopy capabilities.



5. Gas-Phase Chemical Physics

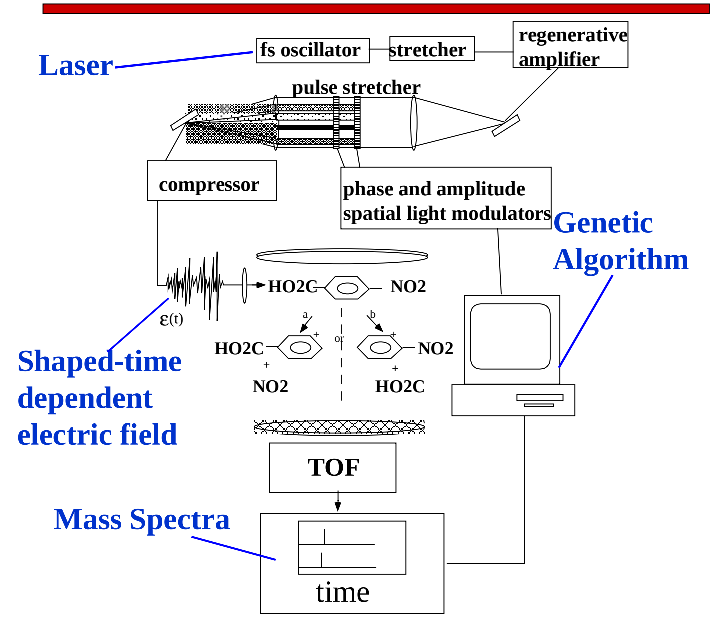
Frontiers of gas-phase chemical physics

Control of photochemistry using shaped pulses: Optical control of chemical reactivity is at the forefront of scientific investigation. Applications in biotechnology and materials chemistry are anticipated. In principle, one could perform photochemistry in a living cell, for example to produce signaling molecules to modify cell function. Precursor molecules might be introduced into the cell which could be modified photochemically after transport through the cell membrane. It is worth noting that IR FEL diagnostics of cell chemistry is currently used in state of-the-art disease monitoring.

Experiments: Preliminary gas-phase experiments are critical for determining the parameters necessary for successful shaped-pulse control of chemical reactions. Particularly, investigation of the limits of shaped-pulse photochemistry of simple chemical systems, such as functionalized organic molecules, will lay the groundwork for extension to complex systems.

Currently, experiments must be done in the strong-field regime; the use of FELs would enable both selection of the center wavelength in strong-field experiments (e.g., to take advantage of regions of transparency in biological applications) as well as allowing extension to the weak-field regime utilizing molecular resonances. Tunable coherent sources offer a unique capability for investigating control in model systems with the capacity for extension to realistic systems (because of the wide range of possible

Quantum Control via Shaped Pulses



wavelengths and high powers). Nonlinear methods provide spatial selectivity since the process occurs only in the high-energy focus of the beam.

Dynamics up to the dissociation limit: The chemistry of ground-state molecules with narrowly defined and tunable energies can be investigated using excitation with successive chirped pulses. Energy-resolved reactivity of molecules is a critical parameter for modeling complex chemical systems, including isomerization, dissociation, and collisional energy transfer. Preparation of tunable microcanonical distributions would provide an unprecedented level of detail for studying and understanding unimolecular reactions.

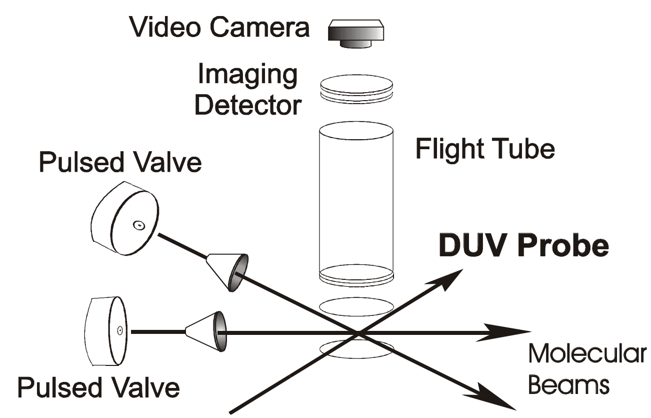
Experiments: The high power and broad tunability of the FEL would enable vibrationally selective chemistry using excitation of modes not accessible with table-top systems. In addition, high-intensity shaped pulses or direct absorption in overtone regions can be used to selectively excite modes that are not currently accessible.

Chirped pulses can completely transfer population (by the phenomenon of rapid adiabatic passage) in a single mode such as a C-H stretch. Within this mode, anharmonicity would prevent overtone excitation. Furthermore, successive pulses, applied after the time scale for internal vibrational redistribution, could be used to continually increase the total energy by single-excitation energy steps. Use of the “optical centrifuge” techniques would further enable high vibrational energy and high rotational energy to be specified independently. In a seeded beam, with polarized excitation, this would in principle allow complete $E_{vibration}$, J, E_{trans}, and alignment control.

First experiments would characterize the excitation efficiency and energy spread as a function of operating parameters such as photon energy, power, and chirp. For example, one could tune the internal energy of a molecule such as ketene over a known threshold for dissociation, and observe the PHOFEX spectrum. As an example of an application, the influence of internal energy on surface reactivity and chemisorption could be studied by scattering the beams of energy-resolved molecules from surfaces.

PHOFEX: Photo-Fragment EXcitation spectroscopy

Single-molecule photoionization: The key reactive species in macroscopic chemical systems (combustion, atmospheric, polymer growth, interstellar chemistry) are molecular radicals, but their inherent reactivity makes them difficult to prepare and study under well-defined conditions. Furthermore, multiple excited potential energy surfaces are often accessed in the course of radical reactions. At the forefront of theoretical and experimental inquiry are nonadiabatic dynamics and underlying factors controlling product branching, angular momentum, and energy disposal. The study of radical-molecule reaction dynamics in crossed beams promises detailed insight into these issues, but is beyond the capability of present-day probe techniques. Similar methods can be used to probe complex kinetics in multicomponent systems. The frontier of chemical kinetic investigations is the study of interacting systems of chemical reactions, whether in atmospheric, combustion, or industrial processing applications.



Single Molecule Photoionization

Experiments: At least three experiments will benefit from a thrust for unit efficiency selective detection:

1. Detection from crossed-beam reactions or sampled chemical reactors or flames (OH+hydrocarbons…).

2. Shaped-pulse and nonlinear detection methods for selectivity.

3. Coincidence with femtosecond pump-probe time-resolved photoelectrons. Experiments require time-synchronized multiple-wavelength capability.

The high flux will also allow these coincidence techniques, which require very efficient detection for all channels, to be used for neutral systems, such as molecular isomerization, photodissociation, and electronic relaxation.

There is a need for a better characterization of basic deep-UV and VUV molecular spectroscopy and photochemistry on which these selective detection schemes are based.

Developing these new techniques also requires understanding of the fundamental nonlinear VUV-XUV photophysics in molecules. This basic knowledge has not been available without intense tunable DUV and VUV sources. In addition, new analytical and chemical dynamics detection techniques can be envisioned using shaped pulses to selectively ionize molecules without fragmentation. Such a capability would dramatically enhance the present ability to investigate reactions using isomer-specific detection.

Time-dependent structural dynamics of molecular transformations: A molecular-level understanding of time-dependent conformational changes will be required for rational design of molecular structures for advanced technological applications. Examples include information transduction by nuclear rearrangement in biological systems, molecular computing, and solar energy conversion. Time-resolved x-ray diffraction will provide a new window on such chemical reactions. The goal is to map nuclear configurations as a chemical reaction proceeds. In biological systems, information transduction often occurs by nuclear rearrangement after photoexcitation.

Experiments: Potential experiments include photoisomerization of a well-studied molecule such as stilbene, followed by a time-dependent probe using x-ray diffraction to establish the utility of the technique. Interesting extensions of this technology would include prototypical vision reactions using retinal. Ring-opening reactions could also be investigated for application in organic reaction mechanisms. Success would bring a powerful tool for investigating time-resolved nuclear motions more directly than ever before. Many experiments which presently "follow" nuclear motion are forced to monitor surrogate properties, which limits applicability to systems where this surrogacy can be well modeled. Direct pair correlations would permit a much broader extension to new systems.

Impact of gas-phase chemical physics research on science, technology, and society

Careful control of photomediated synthesis and fabrication, using feedback optimization of photochemistry, allows for the design of smart materials and the photofabrication of nanodevices and novel and complex materials. Other examples include nuclear rearrangements in biosystems, molecular computing, and solar energy conversion. Another long-term payoff is the ability to perform controlled photochemistry in a living cell.

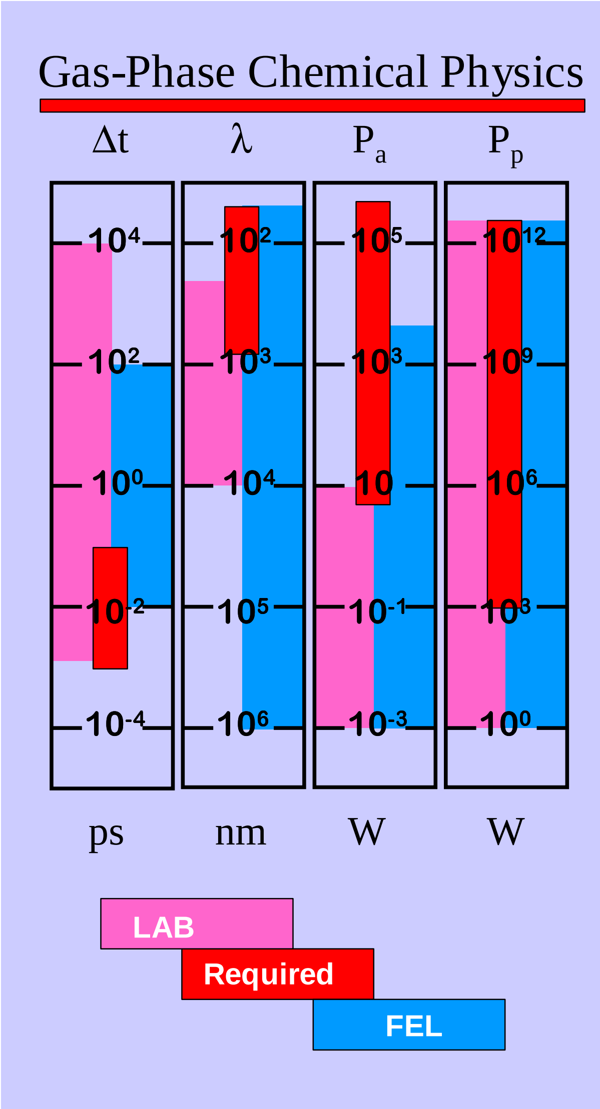
Source requirements for gas-phase chemical physics.

Experiments in photochemical control require large-bandwidth pulses for making a wide range of Fourier components to coherently and simultaneously drive many molecular modes. In a genetic optimization algorithm this amounts to a larger gene pool to control pulse shaping. A consistent phase relationship must be present in the pulses.

Strong-field experiments require intensities on the order of 10^{13} W/cm^2 and the time scale of picoseconds to control nuclear motion. Common to all applications is a requirement for reproducible pulse-to-pulse position and amplitude stability. New developments in state-of-the art pulse-shaping technology for FELs may be needed to fully exploit the capability for coherent control.

The dissociation limit dynamics experiments require tunable high-intensity IR pulses which can be swept in frequency during the pulse as well as slowly varying the frequency of successive pulses. Tunability is essential to allow selection of vibrational modes. The repetition rate must be chosen to match molecular and experimental characteristics.

The single-molecule photoionization experiments require a tunable VUV (8–20 eV) flux of 10^{19} /sec and a bandwidth of 10^{-3}–10^{-4}. Coincidence experiments will require high repetition rates and high detection efficiency. The laser must deliver synchronized (to



subpicosecond) independently tunable multiple-wavelength (DUV to IR) femtosecond pulses at high repetition.

Finally, the time-dependent structural dynamics studies require an intense narrow-bandwidth x-ray pulse that is synchronized with an intense NIR-to-visible pump pulse.

Conclusions

In science, new tools can drive new science, the telescope being a classic example. Scientific needs can also drive the creation of new tools. The invention of the laser helped to change the nature of many scientific fields while the needs of the scientists have motivated pushing laser technology to new limits. Into this scenario have come new free-electron lasers that have new capabilities that hold the possibility to drive science at the cutting edge. The purpose of this workshop was to identify the science that would benefit most from the capabilities of the existing new FELS and would drive the creation of new capabilities for future lasers.

We believe that an opportunity exists for the USA to maintain a world-leading position by developing a new generation of FEL user facilities in the far-IR–to–VUV region. The technology now exists to satisfy many of the scientific demands in this photon energy range, and new technological advances are opening doors daily. The next generation of FELs can provide data in a region of parameter space not previously obtainable. Obtaining data in regions previously inaccessible is a primary way of shifting scientific paradigms. The next generation of FELs will achieve new records in peak power to drive nonlinear processes, wide tunability to search for optimal wavelengths or map out the energy dependence of processes, and very short time-scale pulses to better couple energy into a system and to allow the measurement of very short time-scale events. Prototype experiments are crucial for the present stage of development of FELs; models emanating from this data must provide a predictive framework for the future as well as consolidate and provide coherence to existing data.

Accelerator-based laser facilities bring novel laser capabilities to broad, multidisciplinary teams. Such environments provide fertile ground for revolutionary breakthroughs in fundamental and applied problems with a great impact on science, technology, and society. As with synchrotron radiation and other national facilities, new models are needed for funding these broadly interdisciplinary devices and the substantial infrastructure that must accompany them.

Here we have presented some ideas of new science that can, in part, be done with present FELs and modest upgrades—some science that will require new capabilities, but capabilities that are achievable with existing technology, and some that will require focused development of new technologies. By putting forth the science, we hope to better coordinate the technological developments with the scientific opportunities, to convince a larger community that FELs can play a unique role in producing photons, and to better understand how FELs fit within the vast array of technologies that provide photons for science, both now and in the future.

Appendix A – Objective and Charge to the Participants

Objective

The goal of this workshop was to identify the scientific questions that will drive the development of intense photon sources in the IR through UV during the coming decade. The workshop brought together experts in materials science, biology, chemistry, surfaces, atomic and molecular physics, medicine, and industrial applications.

Several free-electron lasers (FELs) are now operating reliably, and, with the developments in table-top lasers and associated instrumentation in the past decade, it is timely to focus on the scientific driving forces that guide the operation and development of bright photon sources. In particular, it may be possible to create sources of specific characteristics to solve critical problems by employing new technologies associated with FELs or conventional lasers.

Charge to the Participants

We reproduce the charge by Pat Dehmer to attendees of a recent workshop at the Advanced Light Source. We have modified point 4.

1. Where is the forefront of your discipline?
2. What can be done to change the way people think about the most fundamental problems in your field? To cause a paradigm shift?
3. By addressing these fundamental problems, what might be the impacts on science broadly? On technology? And on society?
4. And, finally, what roles do high-brightness photon beams play in addressing these scientific challenges and what source characteristics are needed?

Appendix A – Objective and Charge to the Participants

Comments:

1. Specific key and new scientific questions must be addressed. It is blatantly insufficient to argue for continuing to do stamp collecting with state-of-the-art facilities.

2. It is not adequate to make a case based on arguments that say something like, with a 10 W laser we can do the following, so with a 100 W laser we could do better. If there are important experiments that are limited by present capabilities, such as brightness, repetition rate, pulse structure, or tunability, these are the type of examples we seek.

3. The workshop will confine itself to photon energies <100 eV, and the emphasis will be on photon energies <10 eV.

4. The workshop will focus on identifying key scientific questions and their technological implications. The identification of these questions should not be limited by a view of what is technologically possible. The goal is to identify the science and let the scientific questions drive the development of new, not-yet-available technology.

Appendix B -- Working Groups

Group 1 – Biomedical Sciences & Technology

Biological physics subgroup
Hans Frauenfelder – Los Alamos National Laboratory (Co-Chair)
Glenn Edwards – Duke University (Co-Chair)
Bob Austin – Princeton University
David Piston – Vanderbilt University

Medical subgroup
Frank Carroll – Vanderbilt University (Chair)
Rox Anderson – Harvard University & Massachusetts General Hospital
Leon Partain – Vanderbilt University Medical Center
Jim Snapper – Glaxo-Wellcome, Inc.
John Sutherland – Brookhaven National Laboratory

Group 2 – Atomic and Molecular Science

William Cooke – The College of William & Mary (Chair)
Margaret Murnane – JILA
Toshiki Tajima – Lawrence Livermore National Laboratory
Nora Berrah – Western Michigan University
Ian Harrison – University of Virginia

Appendix B - Working Groups

Group 3 – Condensed Phase Dynamics

Norman Tolk – Vanderbilt University (Chair)
Alan Schwettman – Stanford University
Jim Allen – University of California, Santa Barbara
Philippe Guyot-Sionnest – University of Chicago
David Citrin – Washington State University
Kirk Rector – Los Alamos National Lab
Christopher Bardeen – University of Illinois
Toni Taylor – Los Alamos National Lab

Group 4 – Nanofabrication and Growth Characterization

Richard Haglund, Jr. – Vanderbilt University (Chair)
Bob Nemanich – NCSU
Alberto Pique – NRL
Dennis Hall – Vanderbilt University
Brian Holloway – The College of William & Mary
Ed Gillman – NSU

5 – Gas-Phase Chemical Physics

Trevor Sears – Brookhaven National Laboratory (Chair)
Arthur Suits – SUNY, Stony Brook
Mike Heaven – Emory University
Craig Taatjes – Sandia National Laboratories
Kevin Lehmann – Princeton University
Robert Levis – Wayne State University

Appendix B - Working Groups

Executive Committee

Jack Crow – Florida State University
Charles Duke – Xerox Corporation
Allan Bromley – Yale University
Tom Theis – IBM

Workshop Support

Ben Craft – CAMD
Fred Dylla – Jefferson Lab
David Ernst – SURA
Erik Johnson – Brookhaven National Laboratory
Sam Krinsky – Brookhaven National Laboratory
George Neil – Jefferson Lab
Eric Rohlfing - DoE
Gwyn Williams –Jefferson Lab

Leslie Swindells – SURA
Cela Callaghan – Jefferson Lab
Donna Gilchrist – Jefferson Lab

Appendix C - Schedule

Wednesday, October 11th

7:00–9:00 Reception, Wyndham Hotel; hors d'oeuvres 7–9 p.m., cash bar.

Thursday, October 12

Location: Wyndham Hotel all day

8:00–9:00	Breakfast for participants, downstairs from lobby.	
9:00	Opening remarks.	
	Department of Energy perspective	Eric Rohlfing
9:15	Charge to the Workshop Participants	Gwyn Williams
9:30	Break into six working groups	
12:00	Lunch	
1:30-5:00	Working groups	
7:00	Dinner	

Friday, October 13

Location: AAAS Building, all day

8:00	Breakfast – AAAS Bldg., 2nd floor.	
9:00	Working groups	
11:00	Working groups start report preparation	
12:00	Lunch – AAAS Bldg., 2nd Floor	
1:00	Working groups continue report preparation	
2:30	Break	
3:00	Charge to the Executive Session	David Ernst
3:15	Reports from the six working groups	
4:30	Meeting of the Executive Committee	
5:30	Responses from the Executive Committee	
6:00	Adjourn	

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